Design of Parallel and High-Performance Computing: 
Distributed-Memory Models and Algorithms

Edgar Solomonik

ETH Zürich

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Summary

Lecture overview

- Review: $\alpha$-$\beta$ communication cost model
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- LogP model: short message broadcast
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- Bulk Synchronous Parallel (BSP) model
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- Bulk Synchronous Parallel (BSP) model
- PGAS languages / one-sided communication
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- Overview and final comments
A simple model for point-to-point messages

The cost of sending a message of size $s$ bytes from one processor to any other is

$$\alpha + s \cdot \beta$$

The latency (per message) cost is $\alpha$, while the inverse bandwidth (per byte) cost is $\beta$. 

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What is the cost if the $i$th processor sends a message of size $s$ to the $(i+1)$th processor for $i \in [1, p]$?

- it depends on whether the messages are dependent!
- the 'total work' is $p \cdot (\alpha + s \cdot \beta)$
- the parallel execution (critical path) cost if the messages are sent simultaneously is only $\alpha + s \cdot \beta$
- the parallel execution (critical path) cost if the messages are sent in sequence is $p \cdot (\alpha + s \cdot \beta)$
Small message broadcasts in the $\alpha$-$\beta$ model

The cost of a binary tree broadcast of a message of size $s$ is

$$2(\log_2(p+1) - 1) \cdot (\alpha + s \cdot \beta)$$
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The LogP model

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- assumes both sender and receiver block until completion
- precludes overlap between multiple messages or between computation and communication
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The LogP model (Culler et al. 1996) enables modelling of overlap for the transfer of a fixed-size message

- $L$ – network **latency** cost (processor not occupied)
- $o$ – sender/receiver sequential messaging **overhead** (processor occupied)
- $g$ – inverse injection rate, i.e. **gap** between messages (processor not occupied)
- $P$ – number of **processors**
Messaging in the LogP model
Small-message broadcasts in the LogP model

Same idea as binomial tree, forward message as soon as it is received, keep forwarding until all nodes obtain it (Karp et al. 1993)
The LogGP model

The parameter $g$ in the LogP model is associated with an implicit packet size

- this injection rate implies a fixed-sized packet can be sent anywhere after a time interval of $g$
- modern computer networks do not have a small fixed packet size and achieve higher bandwidth for large messages
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The LogGP model (Alexandrov et al. 1997) introduces another bandwidth parameter $G$, which dictates the bandwidth achieved by large point-to-point messages

- $g$ – gap; minimum time interval between consecutive message transmissions
- $G$ – Gap per byte; time per byte for a long message
The LogGP model

Large-message broadcasts

Lets now consider broadcasts of a message of a large size $s$ (we will assume $s \geq P$)
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- the goal is to get as close as possible to (in the $\alpha$-$\beta$ model sense) a bandwidth cost of $s \cdot \beta$
- binomial tree is very bad, root sends message $\log(p)$ times, i.e. the cost is approximately
  \[ \log(p) \cdot s \cdot \beta \]
Pipelined binary tree broadcast

Send a fixed-size packet to left child then to right child (entire message of size $s$)

- the LogP model has a fixed packet size $k_{\text{LogP}}$ associated with $g$ and yields the cost

$$T_{\text{PBT}}^{\text{LogP}} \approx \log(P) \cdot (L + 3 \max(o, g)) + 2(s/k_{\text{LogP}}) \cdot \max(o, g)$$
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- in the LogGP model we can select a packet size $k$ and obtain the cost

$$T_{\text{PBT}}^{\text{LogGP}}(k) \approx \log(P) \cdot (L + 3 \max(o, g) + 2G \cdot k) + 2(s/k) \cdot (\max(o, g) + G \cdot k)$$

minimizing the packet size $k$, $T_{\text{PBT}}^{\text{LogGP}}(k_{\text{opt}}) = \min_k T_{\text{PBT}}^{\text{LogGP}}(k)$ (via e.g. differentiation by $k$) we obtain the optimal packet size

$$k_{\text{opt}}^{\text{LogGP}} = \sqrt{s/\log(P)} \cdot \sqrt{\frac{\max(o, g)}{G}}$$

so the best packet size, depends not only on architectural parameters, but also on dynamic parameters: the number of processors and message size
Pipelined binary tree broadcast contd.

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- in the $\alpha$-$\beta$ model for a packet size of $k$, we obtain the cost

\[ T^{\alpha, \beta}_{\text{PBT}}(k) \approx 2(\log(P) + s/k)(\alpha + k \cdot \beta) \]

with a minimal packet size of

\[ k_{\text{opt}}^{\alpha, \beta} = \sqrt{s/\log(P)} \cdot \sqrt{\frac{\alpha}{\beta}} \]
Pipelined binary tree broadcast conclusions

The LogP model is inflexible, while the LogGP and the $\alpha$-$\beta$ models capture the key input and architectural scaling dependence

$$T_{\text{PBT}}^{\alpha,\beta}(k) \approx 2(\log(P) + s/k)(\alpha + k \cdot \beta)$$

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Q: Could we get rid of the factor of two constant in the $O(s \cdot \beta)$ cost?

A: Not so long as the root sends two copies of the whole message...
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The minimized cost in the $\alpha$-$\beta$ model is

$$T_{\text{PBT}}^{\alpha,\beta}(k_{\text{opt}}^{\alpha,\beta}) \approx 2\left(\log(P) + \sqrt{s \cdot \log(P)} \cdot \sqrt{\frac{\beta}{\alpha}}\right) \cdot \left(\alpha + \sqrt{\frac{s}{\log(P)} \cdot \sqrt{\alpha \cdot \beta}}\right)$$

$$\approx 2 \log(P) \cdot \alpha + \sqrt{2s \cdot \log(P)} \cdot \sqrt{\alpha \cdot \beta} + 2s \cdot \beta$$
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Double Tree (not the Hilton hotel chain, but still fancy)

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Idea of Double Pipelined Binary Tree: use two binary trees, where every non-root processor is a leaf in one and an internal node in the other, send half of the message down each tree.
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Double pipelined binary tree

The cost of the double pipelined binary tree is essentially the same as the cost of a single pipelined binary tree with half the message size,

\[ T_{DPBT} \approx 2 \log(P) \cdot \alpha + \sqrt{s \cdot \log(P)} \cdot \sqrt{\alpha \cdot \beta} + s \cdot \beta \]

for a sufficiently large message size \((s)\) this is twice as fast as a single pipelined binary tree
Other types of collective communication

We can classify collectives into four categories

- **One-to-All**: Broadcast, Scatter
- **All-to-One**: Reduce, Gather
- **All-to-One + One-to-All**: Allreduce (Reduce + Broadcast), Allgather (Gather + Broadcast), Reduce-Scatter (Reduce + Scatter), Scan
- **All-to-All**: All-to-all

MPI (Message-Passing Interface) provides all of these as well as variable size versions (e.g. (All)Gatherv, All-to-allv), see online for specification of each routine
Tree collectives

We have demonstrated how (double/pipelined) binary trees and binomial trees can be used for broadcasts

- A reduction may be done via any broadcast tree with the same communication cost, with reverse data flow

$$T_{\text{reduce}} = T_{\text{broadcast}} + \text{cost of local reduction work}$$
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Scatter is strictly easier than broadcast, pipeline half message to each child in a binary tree

\[ T_{\text{scatter}} \approx 2 \log(P) \cdot \alpha + s \cdot \beta \]

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\[ T_{\text{gather}} = T_{\text{scatter}} \]
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**All-to-One + One-to-All** collectives can be done via two trees, but is this most efficient? What about **All-to-All** collectives?
Butterfly network
Butterfly network
Butterfly Allgathering (recursive doubling)
Cost of butterfly Allgather

The butterfly has $\log(p)$ levels. The size of the message doubles at each level until all $s$ elements are gathered, so the total cost is

$$T_{\text{allgather}} = \alpha \cdot \log(p) + \beta \cdot \sum_{i=1}^{\log(p)} \frac{s}{2^i} = \alpha \cdot \log(p) + \beta \cdot s$$

The geometric summation in the cost is typical of butterfly algorithms and critical to their efficiency.

- no pipelining necessary to get rid of $\log(p)$ factor on bandwidth cost!
Butterfly Reduce-Scatter (recursive halving)
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\[ T_{\text{reduce-scatter}} = T_{\text{allgather}} + \text{cost of local reduction work} \]
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Butterfly Allreduce: note recursive structure of butterfly

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Its possible to do Scan (each processor ends up with a unique value of a prefix sum rather than the full sum) in a similar fashion, but also with operator application done additionally during recursive doubling (Allgather)
Butterfly Scatter

Question: Which tree is this equivalent to?
Butterfly Broadcast
Butterfly Broadcast

\[ T_{\text{broadcast}} = T_{\text{scatter}} + T_{\text{allgather}} \]
Butterfly Gather

Question: Which other butterfly collective can utilize Gather as a subroutine?
Collectives Protocols for Large Messages

Butterfly Reduce

\[ T_{\text{reduce}} = T_{\text{reduce-scatter}} + T_{\text{gather}} \]
Butterfly Reduce

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Butterfly All-to-All

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Note that the size of the message stays the same at each level:

$$\text{All-to-All} = \alpha \cdot \log(p) + \beta \cdot \log(p)$$

It's possible to do All-to-All in less bandwidth cost (as low as \(\beta \cdot s\) by sending directly to targets) at the cost of more messages (as high as \(\alpha \cdot p\) if sending directly).
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\[
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**BSP model definition**

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- Execution is subdivided into supersteps, each associated with a global synchronization.
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- we will focus on a variant of BSP with $h = p$ and for consistency refer to $\hat{g}$ as $\beta$ and the cost of a synchronization as $\alpha$
Synchronization vs latency

By picking $h = p$, we allow a global barrier to execute in the same time as the point-to-point latency

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- collectives can be done in linear bandwidth cost with $O(1)$ supersteps
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- Enables high-level algorithm development: how many collective protocols does the algorithm need to execute?
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- enables high-level algorithm development: how many collective protocols does the algorithm need to execute?
- global barrier may be a barrier of a subset of processors, if BSP is used recursively
Nonblocking communication

The paradigm of sending non-blocking messages then synchronizing later is sensible

- MPI provides non-blocking 'I(send/recv)' primitives that may be 'Wait'ed on in bulk (these are slightly slower than blocking primitives, due to buffering)
- MPI and other communication frameworks also provide one-sided messaging primitives which are zero-copy (no buffering) and very efficient
- one-sided communication progress must be guaranteed by a barrier on all or a subset of processors (or MPI Win Flush between a pair)
(Reduce-)Scatter and (All)Gather in BSP

When \( h = p \) all discussed collectives that require a single butterfly can be done in time \( T_{\text{butterfly}} = \alpha + s \cdot \beta \) i.e. they can all be done in one superstep

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When \( h = p \) all discussed collectives that require a single butterfly can be done in time \( T_{\text{butterfly}} = \alpha + s \cdot \beta \) i.e. they can all be done in one superstep

- Scatter: root sends each message to its target (root incurs \( s \cdot \beta \) send bandwidth)
- Reduce-Scatter: each processor sends its portion to every other processor (every processor incurs \( s \cdot \beta \) send and receive bandwidth)
- Gather: send each message to root (root incurs \( s \cdot \beta \) receive bandwidth)
- Allgather: each processor sends its portion to every other processor (every processor incurs \( s \cdot \beta \) send and receive bandwidth)

when \( h < p \), we could perform the above algorithms using a butterfly with ‘radix’ = \( h \) (number of neighbors at each butterfly level) in time

\[
T_{\text{butterfly}} = \log_h(p) \cdot \alpha + s \cdot \beta
\]
Other collectives in BSP

The Broadcast, Reduce, and Allreduce collectives may be done as combinations of collectives in the same way as with Butterfly algorithms, using two supersteps

- Broadcast done by Scatter then Allgather
- Reduce done by Reduce-Scatter then Gather
- Allreduce done by Reduce-Scatter then Allgather

Sign of a good model: simpler, yet preserves qualitative results
Other collectives in BSP

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However, (bad sign) BSP with $h = p$ can do all-to-all in $O(s)$ bandwidth and $O(1)$ supersteps (as cheap as other collectives), when $h < p$, the logarithmic factor on the bandwidth is recovered.
Systems for one-sided communication

BSP employs the concept of non-blocking communication, which presents practical challenges

- to avoid buffering or additional latency overhead, the communicating processor must know or be aware of the desired buffer location of the remote processor
- if the location of the remote buffer is known, the communication is called 'one-sided'
- with network hardware known as Remote Direct Memory Access (RDMA) one-sided communication can be accomplished without disturbing the work of the remote processor

One-sided communication transfers are commonly be formulated as

- 'Put' – send a message to a remote buffer
- 'Get' – receive a message from a remote buffer
Partitioned Global Address Space (PGAS)

PGAS programming models facilitate non-blocking remote memory access:
- they allow declaration of buffers in a globally-addressable space, which other processors can access remotely.
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- MPI supports one-sided communication via declaration of ’windows’ that declare remotely-accessible buffers.
Matrix multiplication

Matrix multiplication of $n$-by-$n$ matrices $A$ and $B$ into $C$, $C = A \cdot B$ is defined as, for all $i, j$,

$$C[i, j] = \sum_k A[i, k] \cdot B[k, j]$$

A standard approach to parallelization of matrix multiplication is commonly referred to as SUMMA (Agarwal et al 1995, Van De Geijn et al 1997), which uses a 2D processor grid, so blocks $A_{lm}$, $B_{lm}$, and $C_{lm}$ are owned by processor $P[l, m]$

- **SUMMA variant 1**: iterate for $k = 1$ to $\sqrt{p}$ and for all $i, j \in [1, \sqrt{p}]$
  - broadcast $A_{ik}$ to $P[i, :]$
  - broadcast $B_{kj}$ to $P[:, j]$
  - compute $C_{ij} = C_{ij} + A_{ik} \cdot B_{kj}$ with processor $P[i, j]$
SUMMA algorithm

\[ T_{\text{SUMMA}} = \sqrt{p} \cdot \left( 2 \log(p) \cdot \alpha + \frac{2n^2}{p} \cdot \beta \right) = 2\sqrt{p} \cdot \log(p) \cdot \alpha + \frac{2n^2}{\sqrt{p}} \cdot \beta \]
3D Matrix multiplication algorithm

Reference: Agarwal et al 1995 and others

\[ T_{3D-MM} = 2 \log(p) \cdot \alpha + \frac{3n^2}{p^{2/3}} \cdot \beta \]
LU factorization

The LU factorization algorithm provides a stable (when combined with pivoting) replacement for computing the inverse of a $n$-by-$n$ matrix $A$,

$$A = L \cdot U$$

where $L$ is lower-triangular and $U$ is upper-triangular is computed via Gaussian elimination: for $k = 1$ to $n$,

- set $L[k, k] = 1$ and $U[k, k : n] = A[k, k : n]$
- divide $L[k+1 : n, k] = A[k+1 : n, k]/U[k, k]$
- update Schur complement

$$A[k+1 : n, k+1 : n] = A[k+1 : n, k+1 : n] - L[k+1 : n, k] \cdot U[k, k+1 : n]$$

this algorithm can be blocked analogously to matrix multiplication
Blocked LU factorization
Blocked LU factorization
Blocked LU factorization
Block-cyclic LU factorization
Block-cyclic LU factorization
Block-cyclic LU factorization

\[ S = A - LU \]
Recursive matrix multiplication

Now let's consider a recursive parallel algorithm for matrix multiplication

\[
\begin{bmatrix}
  C_{11} & C_{12} \\
  C_{21} & C_{22}
\end{bmatrix} =
\begin{bmatrix}
  A_{11} & A_{12} \\
  A_{21} & A_{22}
\end{bmatrix} \cdot
\begin{bmatrix}
  B_{11} & B_{12} \\
  B_{21} & B_{22}
\end{bmatrix}
\]

\[
C_{11} = A_{11} \cdot B_{11} + A_{12} \cdot B_{21}
\]
\[
C_{21} = A_{21} \cdot B_{11} + A_{22} \cdot B_{21}
\]
\[
C_{12} = A_{11} \cdot B_{12} + A_{12} \cdot B_{22}
\]
\[
C_{22} = A_{12} \cdot B_{21} + A_{22} \cdot B_{22}
\]

This requires 8 recursive calls to matrix multiplication of \(n/2\)-by-\(n/2\) matrices, as well as matrix additions at each level, which can be done in linear time.
Recursive matrix multiplication: analysis

If we execute all 8 recursive multiplies in parallel with \( p/8 \) processors, we obtain a cost recurrence of

\[
T_{\text{MM}}(n, p) = T_{\text{MM}}(n/2, p/8) + O\left(\frac{n^2}{p} \cdot \beta\right) + O(\alpha)
\]

The bandwidth cost is dominated by the base cases, where it is proportionate to

\[
(n/2^{\log_8(p)})^2 = (n/p^{\log_8(2)})^2 = (n/p^{1/3})^2 = n^2/p^{2/3}
\]

for a total that we have seen before (3D algorithm)

\[
T_{\text{MM}}(n, p) = O\left(\frac{n^2}{p^{2/3}} \cdot \beta\right) + O(\log(p) \cdot \alpha)
\]
Recursive LU factorization

LU factorization has the form

\[
\begin{bmatrix}
A_{11} & A_{12} \\
A_{21} & A_{22}
\end{bmatrix} =
\begin{bmatrix}
L_{11} & 0 \\
L_{21} & L_{22}
\end{bmatrix} \cdot
\begin{bmatrix}
U_{11} & U_{12} \\
0 & U_{22}
\end{bmatrix}
\]

and can be computed recursively via

\[
\begin{align*}
[L_{11}, U_{11}] &= \text{LU}(A_{11}) \\
L_{21} &= A_{21} \cdot U_{11}^{-1} \\
U_{12} &= L_{11}^{-1} \cdot A_{12} \\
[L_{22}, U_{22}] &= \text{LU}(A_{22} - L_{21} \cdot U_{12})
\end{align*}
\]

The inverses $L_{11}^{-1}$ and $U_{11}^{-1}$ may be obtained as part of the recursion in the first step (see Tiskin 2002 for details). There are two recursive calls to LU and 3 matrix multiplications needed at each step.
Recursive LU factorization: analysis

The two recursive calls within LU factorization must be done in sequence, so we perform them with all the processors. We have to also pay for the cost of matrix multiplications at each level

\[ T_{LU}(n, p) = 2 T_{LU}(n/2, p) + O(T_{MM}(n, p)) \]

\[ = 2 T_{LU}(n/2, p) + O\left(\frac{n^2}{p^{2/3}} \cdot \beta + \log(p) \cdot \alpha\right) \]

with base-case cost (sequential execution)

\[ T_{LU}(n_0, p) = O(n_0^2 \cdot \beta + \log(p) \cdot \alpha) \]

the bandwidth cost goes down at each level and we can execute the base-case sequentially when \( n_0 = n/p^{2/3} \), with a total cost of

\[ T_{LU}(n, p) = O\left(\frac{n^2}{p^{2/3}} \cdot \beta\right) + O(p^{2/3} \cdot \log(p) \cdot \alpha) \]
Conclusion and summary

Summary:

- important parallel communication models: $\alpha$-$\beta$, LogP, LogGP, BSP
- collective communication: binomial trees are good for small-messages, pipelining and/or butterfly needed for large-messages
- collective protocols provide good building blocks for parallel algorithms
- recursion is a thematic approach in communication-efficient algorithms

Next semester:

- Consider taking "Research Topics in Software Engineering" next semester, it will have nothing to do with software engineering and lots to do with theory of parallel computation!
Backup slides
This seminar introduces students to fundamental results in parallel programming and design. Students will study and present research papers that span topics in both theory and practice, ranging from foundations parallel computing to applications. The focus will be on fundamental lower and upper bounds, thus, many papers will be dated. Students need a solid mathematical background.